GEOSTATISTICAL ASSESSMENT OF CONE PENETROMETER TEST DATA FOR SOIL CHARACTERIZATION BASED ON ULTRAVIOLET INDUCED FLUORESCENCE

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ABSTRACT

Site characterization at a hydrocarbon-impacted site was performed using cone penetrometer testing with ultraviolet induced fluorescence (UVIF-CPT). The UVIF-CPT comprises a full piezo cone penetrometer that records tip resistance, sleeve friction, pore pressure and ultraviolet induced fluorescence. Aromatic compounds in petroleum hydrocarbons (PHCs) will fluoresce under ultraviolet light. UVIF-CPT was used to delineate subsurface PHC contamination. Geostatistical methods were then used to assess spatial continuity and uncertainty associated with the geological interpretation based on the CPT data.

The results suggested complex layering of several soil types and thin, discontinuous zones of hydrocarbon impact. Lateral continuity of soil types and/or hydrocarbon-affected zones was not clear. Modelling was based on a variable, Vclay (approximating the fraction of fine-grained soil, hence hydraulic conductivity), based on soil behaviour types interpreted from CPT logs.

A single realization was drawn from multiple simulations with no obvious bias and a reasonably narrow spread in global statistics. The geologic simulation showed thin, laterally continuous, interbedded layers with varying Vclay. Based on the inferred permeability relationship, the model is consistent with thin zones of hydrocarbon impact indicated by the UVIF raw data.

RÉSUMÉ

La caractérisation de site à un site d'hydrocarbure influé a été exécutée en utilisant l'essai de penetrometre de cône avec la fluorescence provoqué par ultraviolet (UVIF CPT). UVIF CPT comprend un penetrometre de cône de piézomètre plein qui enregistre la résistance de pointe, la friction de manche, la pression de pore et la fluorescence provoqué par ultraviolet. Les composés aromatiques dans les hydrocarbures de pétrole (PHCs) seront fluorescents sous la lumière ultraviolette. UVIF CPT a été utilisé pour délinéer la contamination de PHC souterrain. Les méthodes géostatistiques ont été alors utilisées pour évaluer la continuité et l'incertitude spatiales associées avec l'interprétation géologique basée sur les données de CPT.

Les résultats suggérent plusieurs couches complexes de plusieurs types de sol et des zones d'impact d'hydrocarbure minces. La continuité entre ces types de sol et ces zones d'hydrocarbure n'était pas evident. Le modelage était basé sur une variable, Vclay (la fraction de sol au grain fin, c'est-à-dire la conductivité hydraulique), basé sur les types de comportement de sol interprétés par des journaux de bord de CPT.

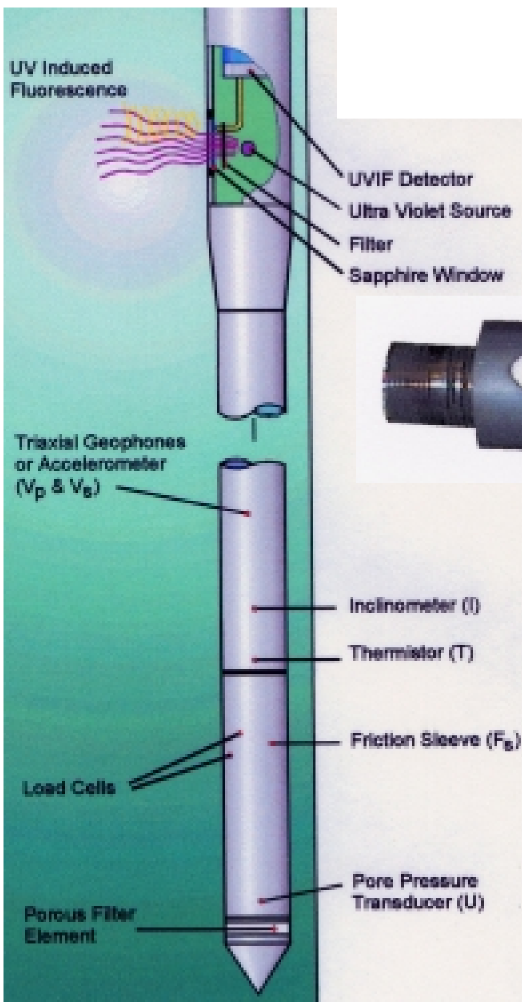
Une seule réalisation a été tirée de plusieurs simulations avec aucun prejugé évident et une diffusion raisonablement étroite dans la statistique globale. La simulation géologique a montré des couches minces, latéralment continues, avec Vclay variable. Selon le rapport de perméabilité, le modèle est en accord avec des zones minces d'hydrocarbure indiqué par les données crues UVIF.

1 INTRODUCTION

1.1 Background

Hydrocarbon impact delineation at contaminated sites is a routine component of environmental site characterization. Ultra violet induced fluorescence (UVIF) cone penetration testing (CPT) can be an efficient approach (Woeller *et al.*, 2003). The CPT was very good at providing detailed insight regarding soil type, changes in soil stratigraphy, the location of the groundwater table along with various soil design parameters. In contrast, the UVIF module successfully detected subsurface hydrocarbon in layers as thin as 0.05 m. At one testsite, multiple UVIF-CPT holes showed widely varying responses within a heterogeneous geologic framework with apparently small-scale vertical and lateral variations.

This paper describes application of geostatistical methods to help characterize geologic uncertainty as a precursor to groundwater flow and contaminant transport modelling at a hydrocarbon-impacted site. The ultimate purpose of modelling is to assess if natural attenuation of petroleum hydrocarbons (PHCs) could mitigate environmental impacts associated with an excavated former flare pit.



This work was completed as part of a larger research effort (Consortium for Research on Natural Attenuation, or CORONA) to assess how natural attenuation can reduce environmental impacts by the upstream oil and gas industry. The overall project includes a geostatistical component, with this paper describing an initial application of using UVIF-CPT data to develop a site conceptual model. Good site characterization is critical when assessing the potential for natural attenuation to manage contaminant plumes.

1.2 UVIF-CPT

Hydrocarbon fluorescence has been used to evaluate cores from oil exploration wells since the 1960's (Riecker, 1962). The UVIF system operates on the principal that aromatic hydrocarbons (containing one or more benzene rings) fluoresce when irradiated by ultra violet light. Therefore, by measuring the UVIF intensity and any spatial changes, one can determine both the lateral and vertical extent of subsurface PHC contamination. A detection limit of approximately 15 mg/kg of dry weight for light nonaqueous phase liquids (LNAPL) in soil is possible according to some researchers (Olie *et al.*, 1994).

The UVIF cone used for this study consists of a piezo cone with a UVIF module, as shown in Figure 1.

During penetration, soil is illuminated with an ultra violet light source through a clear sapphire window. Fluorescence emitted by any aromatics in the soil is detected in the probe by a small photo multiplier tube, and a signal (in Volts) is conducted through the electrical CPT cable to a data processing system in the CPT rig. This approach is simpler than the Laser Induced Fluorescence (LIF) system where fibre-optic cables are required to transmit laser light down and any resulting fluorescence back up to surface to a spectrometric analyzer.

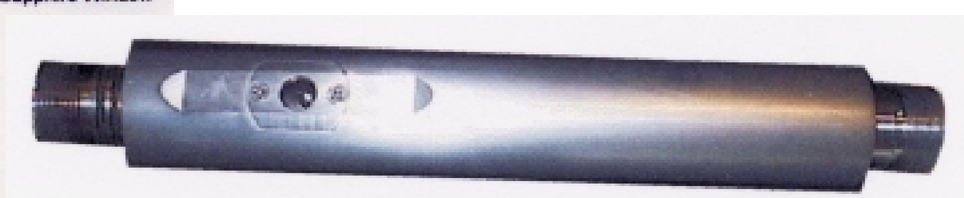


Figure 1 – UVIF-CPT Module

The intensity of contaminant fluorescence (above background levels) depends on both the relative concentration and number of aromatic rings in the compounds. The detection system can be modified to optimize the identification of specific contaminants by using filters to control the emission wavelength recorded.

A typical contaminated site investigation initially focuses on presence and distribution of regulated target compounds, usually because of their potential human health and environmental risk. Compounds of potential concern include the BTEX suite and selected aromatics.

Limiting analysis to typical target compounds can be misleading if it precludes other aromatic compounds that may contain substitutions of sulfur, oxygen, nitrogen, *etc*. for hydrogen atoms in the structure. Such substitutions can result from incomplete combustion of the parent aromatic compound found in the crude oil, or may be microbial metabolites of the parent compound resulting from in-situ biodegradation.

UVIF-CPT has been used to characterize petroleum hydrocarbon presence near several upstream oil and gas sites (Woeller *et al.*, 2003). This paper focusses on geostatistical analysis of the UVIF-CPT data around a former flare pit.

1.3 Geostatistics

Efforts to remediate environmental impacts resulting from industrial activities have lead to increased recognition of the importance of developing a detailed hydrogeological model. At the same time, improved site characterization tools have shown that almost all subsurface environments exhibit substantial variability. The modern approach to dealing with this variability has been increasing use of geostatistical tools to assess and characterize data uncertainty in hydrogeological models. Insight gained about data uncertainty can then be used to help optimize future characterization efforts and gain understanding about groundwater flow and contaminant transport simulations.

2 SITE REVIEW

2.1 Site Description

Initial site characterization was conducted using the solid stem auger method. A series of boreholes were logged and sampled to approximately 5 m below ground surface (mbgs), with 11 completed as monitoring wells. Soil logs indicated a heterogeneous distribution of clay, silt and sandy units. Based on these data, the soil in the immediate flare pit area was excavated to approximately 4-5 mbgs several years before the UVIF-CPT program. Free-phase hydrocarbon was suspected to remain at the site, based on soil testing, but its presence had never been confirmed. Dissolved hydrocarbons were noted in the nearest two wells south of the former pit.

Eighteen UVIF-CPT holes were advanced in two sets (10 in 2001, 8 in 2002). These holes roughly follow a grid pattern south of the former pit. Hole depths ranged from 4 to 10 mbgs, with deeper holes being pushed higher up the hill near the pit. Figure 2 shows a plan map of the CPT holes. The UVIF response was most uniform and highest in magnitude immediately south of the former pit. Further downgradient, responses were increasingly variable in both magnitude and elevation.

The area of hydrocarbon impact is approximately 50m wide by 60m long, with a topographic slope to the south from the hydrocarbon source area (former flare pit). Hydrocarbon impact is noted at depths ranging from approximately 2 to 10 m below ground surface (near the source).

The UVIF-CPT boreholes provide a sequence of depth-discrete measurements (2.5 cm interval) of mechanical and contaminant variables. Each hole provides a depth-measured trace of cone tip resistance, cone sleeve friction, pore pressure response and ultraviolet induced fluorescence (related to presence of free phase hydrocarbon). These data identify both gross scale geologic response and detailed assessment of small-scale fluctuations in soil properties.

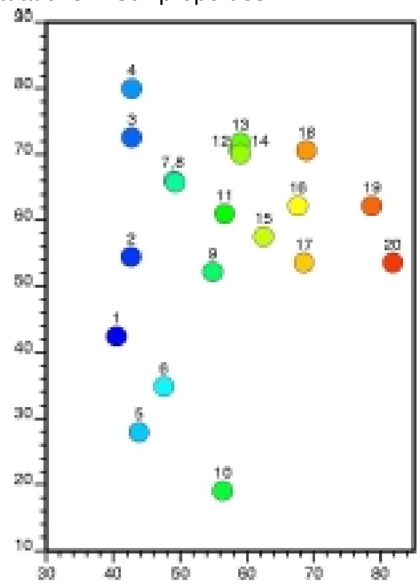


Figure 2 – CPT Hole Locations

The domain for geostatistical modelling was selected as being 50 m wide by 80 m long to incorporate the UVIF-CPT wells. The CPT logs suggested that this domain had a relatively consistent geology comprising mainly silt and clay with some sandy units. The highest hydrocarbon impact was detected in UVIF logs from locations 3, 11, 12, 13, 14 and 16. Minor detections may be present in 9, 15, 17 and 18.

3 GEOSTATISTICAL MODELLING

3.1 Decision of Stationarity

The first step in geostatistical modelling is making the decision of stationarity, comprising selection of the zone of interest and appropriate random variable(s) exhibiting consistent statistical response. This decision is an important factor in successful modelling.

The CPT data comprise a series of strip logs giving depth-specific values for cone tip resistance, sleeve friction, pore pressure and UVIF response. The data are collected every 2.5 cm, but are typically averaged over 0.1 m to account for the property measurement scale. The CPT logs provide a consistent and objective measure of geologic contacts and small-scale features that will not be noted in observation-based geologic logs. CPT-based geologic descriptions are based on correlation charts linking CPT response to soil behaviour type (SBT). The charts are based on empirical data linking SBT through a cross-plot of tip resistance and friction ratio (tip resistance divided by sleeve friction).

The raw CPT data were evaluated for evidence of correlation, but no clear link was evident between the UVIF data and basic CPT logs. The random variable for simulations was therefore based on the interpreted SBT. Most of the SBT ranged from clay (SBT=3) to sand (SBT=9), with a few thin layers classified as stiff, fine-grained soil (SBT=12). A random variable, Vclay (1 to 0), was developed to represent the percent of fine-grained soil particles. Vclay values (Figure 3) were assigned using a step-wise linear transform:

$$Vclay = 1.5 - SBT/6 \qquad \text{Equation 1}$$

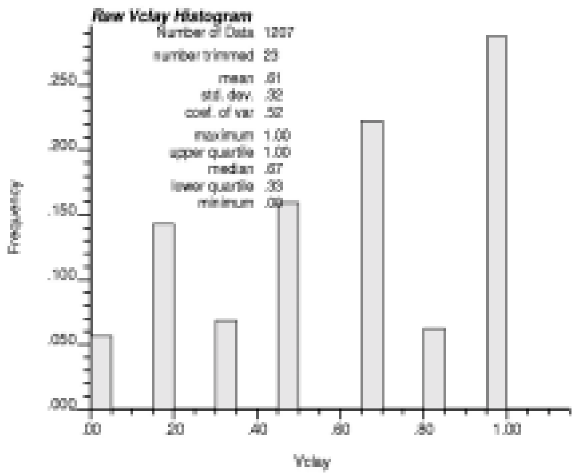


Figure 3 – Histogram of Raw Vclay Data

and then normal-score transformed using GSLIB (Deutsch and Journel, 1998). An external trend in Vclay was noted after plotting averaged values by position and elevation. Figure 4 shows an inferred trend relating Vclay to Northing co-ordinate, and the linear model. The 2001 data are outlined with a square (no outline for 2002 data), while points shown as circles are from the south part of the domain (Northing< 4850).

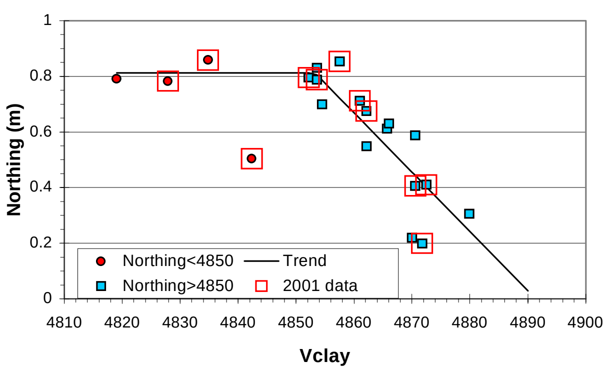


Figure 4 – Vclay Data Trend with Northing Coordinate

The linear model was:
Northing>4852 m, Vclay = 0.8119 (constant)
Northing<4852 m, Vclay = -0.0213(Northing – 4810) + 1.7334 (linear decrease)

Extrapolation was prevented for Northings>4880 because these locations would have a physically unrealistic trend value of Vclay<0.

Variogram modelling (Figure 5) was conducted using the 'residual' set. The set was developed by subtracting the trend value (based on Northing) from each Vclay value, then doing a normal score transformation.

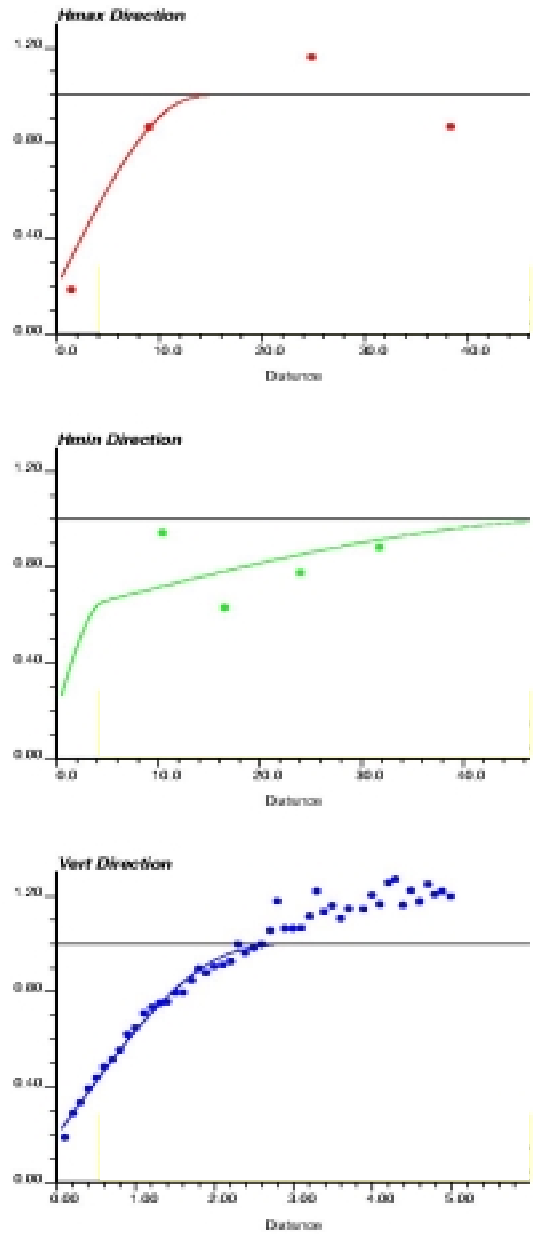


Figure 5 – Data and 3-D Variogram Model

3.2 Experimental Variogram Modelling

Development of the variogram model is the second key component of geostatistical modelling. This model defines the spatial continuity of the random variable in a statistical sense, and forms the basis for subsequent geostatistical simulation. The variogram model involves getting a 'best fit' match of experimental data variograms, using a linear combination of one or more allowed functions. These functions have specific properties vital to the simulation process. Details regarding variogram modelling are provided in Deutsch (2002) and Isaaks and Srivastava (1989).

Variogram modelling was performed in three dimensions using the normal-score transformed residual Vclay data. The model was fitted to the experimental variograms. The final model and experimental variograms plotted on Figure 5 are summarized below.

Variance	Variogram Type	Horiz. Range (N-S)	Horiz. Range (E-W)	Vert. Range
0.2	Nugget			
0.39	Spherical	15.3	54	3.0
0.41	Spherical	12.8	4.6	2.3

The effect of explicitly removing the trend is evident in the Hmin plots, where the data 'see' the full variance.

The model was used as input for cross validation with kriging the data to assess whether the model could adequately reproduce the measured data (*i.e.*, assess uncertainty and unbiasedness in the kriged estimate). Typically measures include checking:

- Scatterplot of true value vs. estimated value (ideally fall on 45^o line);
- Scatterplot of estimate vs. error (estimate-true) (ideally spread equally around 0); and,
- Histogram of error (ideally, mean of 0 and narrow spread).

The results (not provided) showed an acceptable correlation between the simulated and true values (0.45), with no bias (mean error near 0).

4 GEOSTATISTICAL SIMULATION

A series of geostatistical simulations were conducted using SGSIM from GSLIB to generate a series of equiprobable realizations of Vclay. The domain was modelled using 26 x 32 x 50 cells (x, y and z, respectively) with dimensions of 2m x 2m x 0.3 m. Simulations used normal scores data, thus final results required back transformation and trend incorporation to get real-world values.

A single realization was selected for visualization using a three-step process:

- plotting the histogram of transformed Vclay (mean near 0 and variance near 1);
- constructing a Q-Q plot of simulated and input data (form a 45^o line); and,
- comparing the variogram of the realization to the model variogram.

Based on all measures, a simulation (input data and model variograms shown in Figure 6) was selected for visualization. The slightly poorer variogram fit at long distances (lags) is relatively unimportant, given the good fit at shorter lags (more important when reproducing data continuity for simulation purposes).

4.1 Visualization

Model output was post-processed by back-transforming the output from Gaussian space into real-world values then adding in the external trend. These simulated values were then plotted to look for the modelled trend and spatial assessment.

The simulated data gave a reasonable match to the interpreted external trend (Figure 7), and even captures the decrease in average Vclay around local Northing = 40 m.

A series of vertical and horizontal planar sections were plotted in Figures 8 and 9. These plots do not incorporate the topographic decrease of approximately 5 m from north to south. The original contaminant source was located at the north end of the domain (high Northing), extending at least 10 m below ground surface at that location (approximately X-Y Slice 15). Groundwater and hydrocarbon flow is generalized as southward.

The sections generally show three notable features. The trend of decreasing Vclay with increasing Northing appears as a greater proportion of 'cooler' colours in this location. This characteristic is most clearly seen in vertical sections where zones of lower Vclay extend southward in relatively thin horizontal layers separated by thicker layers with high Vclay (clay-rich). In contrast, there is a preponderance of high Vclay zones at the south end of the domain. Finally, the horizontal sections generally show a zone (wedge) of higher Vclay material in the domain middle. Implications of these patterns are discussed below.

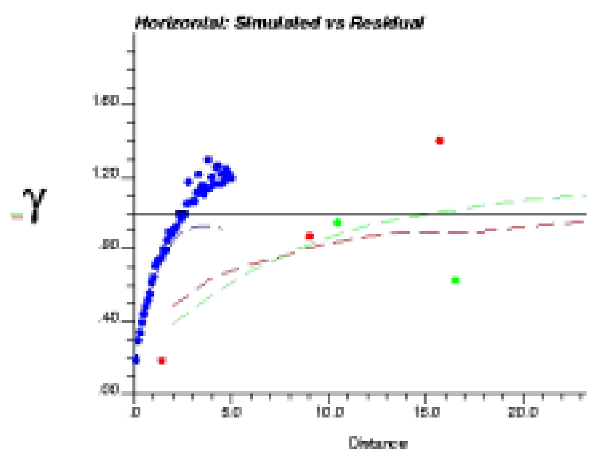


Figure 6 – Variograms for Residual Simulations (normal scores)

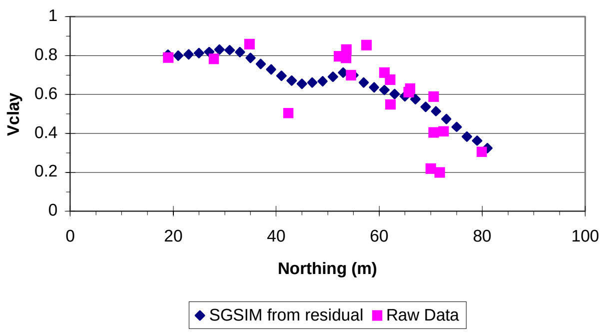


Figure 7 – Model Output Showing External Trend

4.2 Model Implications

The Vclay variable is based on soil behaviour type, hence may have an underlying inverse relationship with permeability. Using this assumption, the simulation sections were reviewed for implications regarding contaminant presence and movement. Hydrocarbon movement, particularly as free-phase liquid, is likely to be controlled by higher permeability units (low Vclay).

The higher proportion of low Vclay soil at the north end (source area) suggests that vertical penetration of hydrocarbon is possible. The characteristic pattern of thin, laterally continuous layers of lower Vclay separated by higher Vclay would be consistent with flow along preferential layers. The zone of higher Vclay in the domain middle may represent a lateral flow barrier and help explain why the plume is restricted to the west side of the area.

5 SUMMARY

The program was intended to evaluate the benefit of using multivariate geostatistical methods with objective UVIF-CPT data to help improve site characterization. The UVIF-CPT data were compiled in a 'clean' database. A continuous random variable, Vclay, was derived based on the soil behaviour type obtained from the CPT data, although no obvious correlation was noted between the CPT logs and UVIF results.

An explicit trend of decreasing Vclay to the north was removed from the Vclay data, and the resulting residual values were used. The work flow involved:

- Normal scores transformation and variogram modelling of the experimental data;
- Kriging with the three-dimensional variogram model, followed by cross validation and accuracy assessment to uncover potential bias;
- Geostatistical modelling using sequential Gaussian simulation to create equi-probable realizations of the domain;
- Assessment to examine reproduction of average domain statistical character;
- Backtransformation of simulations and trend introduction to create a realization in real space Vclay units;

One simulation was selected that appeared best able to reproduce the statistical character of the original data. This simulation reproduced the inferred trend. A qualitative review of the results showed several features that may influence future flow modelling of contaminated groundwater. Assuming that Vclay includes a permeability factor, the model suggested:

- Zones of lower Vclay (higher permeability) showed southward lateral continuity but were vertically separated by layers of higher Vclay (lower permeability);
- Regions of higher Vclay may restrict cross-gradient contaminant spreading; and,
- The domain area downgradient from the contaminant source has higher average Vclay, possibly representing a permeability barrier to plume growth.

Further effort is required to combine the geologic characterization obtained from this program with contaminant flow and transport modelling.

The UVIF-CPT provides another powerful tool in the suite of systems that can be used by the professional to cost-effectively characterize contaminated sites. It was found to provide excellent results in the delineation of PHC contamination emanating from a flare pit associated with oil and gas production. It did not, however, provide the desired resolution when used to track the extent of a natural gas condensate plume. This experience underscores the importance of working with the providers of the UVIF equipment early on during the proposed use of the technology. It is beneficial to have soil samples contaminated with compounds of concern sent to the UVIF providers for preliminary assessment of the response to evaluate if the UVIF system will provide the desired results.

6 REFERENCES

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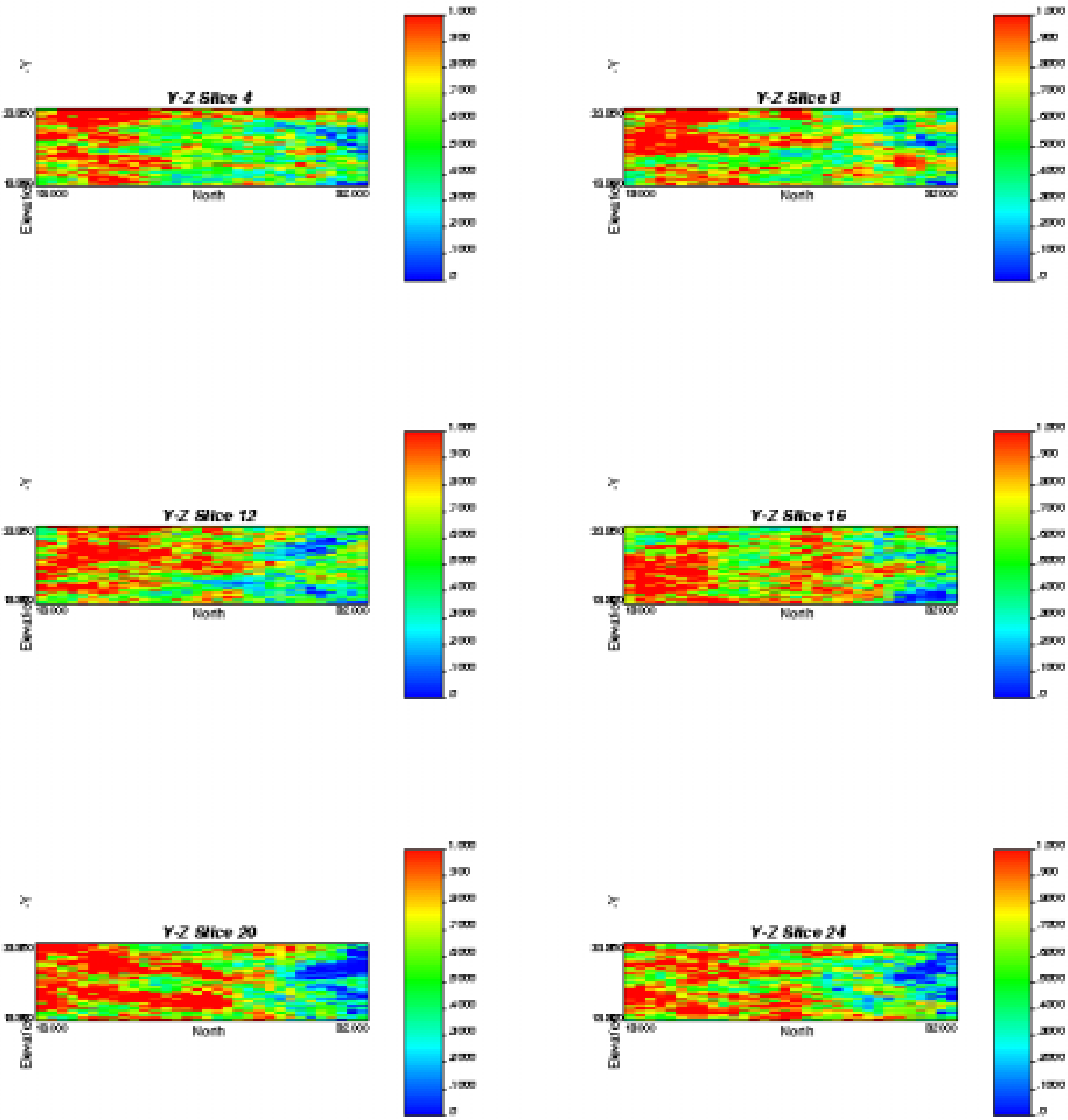

Figure 8 – Selected Vertical Sections Looking West

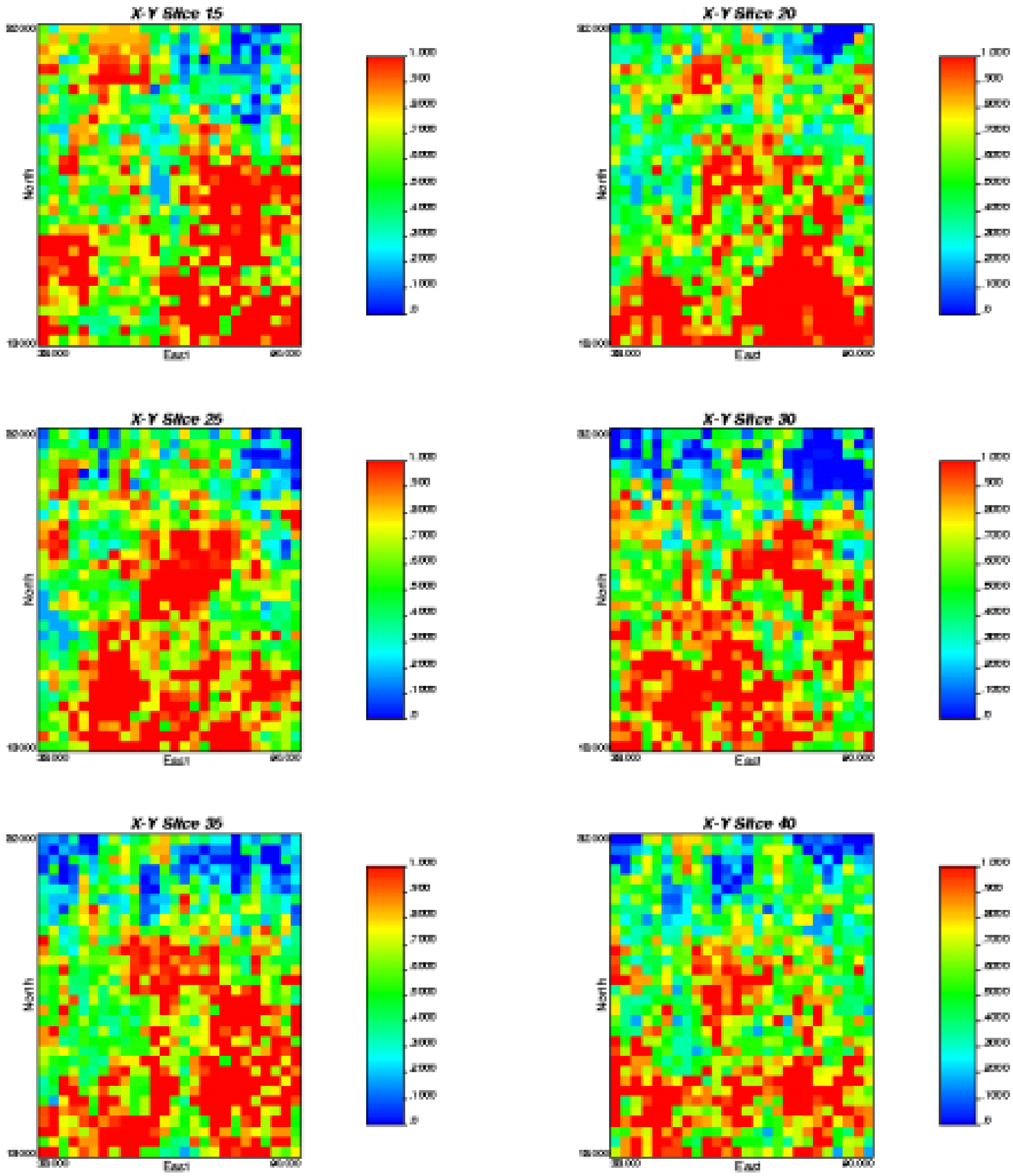

Figure 9 – Selected Horizontal Sections, Simulation 4

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